Thiophene
110-02-1 | DTXSID8026145

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.06e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.69e-01

Confidence level: 8.44e-01

Nearest Neighbors from the Training Set

Image not found
Thiophene
Measured: 3.58e-02
Predicted: 4.06e-02

Image not found
Methyl disulfide
Measured: 3.18e-02
Predicted: 2.94e-02

Image not found
Propargyl bromide
Measured: 1.25e-01
Predicted: 9.48e-02

Image not found
Allyl bromide
Measured: 3.17e-02
Predicted: 4.20e-02

Image not found
1,3-Cyclopentadiene
Measured: 2.72e-02
Predicted: 2.15e-02